The effects of Cup-like and Hill-like Parabolic Confining Potentials on the Photoionization Cross Section in a Spheroidal Quantum Dot

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ABSTRACT

A theoretical investigation of the effects of the hill-like and the cup-like electric confining potentials, both parabolic and superimposed on an infinite spherical square well (ISSW) potential, on the photoionization cross section (PCS) in a spheroidal quantum dot is presented. As the cup-like parabolic potential intensifies, the peak of the PCS becomes red-shifted for the $s \rightarrow p$ transition, and becomes blue-shifted for the $p \rightarrow d$, $d \rightarrow f$ (and so forth) transitions. The hill-like potential, on the contrary, blue shifts the peaks of the PCS for the $s \rightarrow p$ transitions, while it red-shifts those of transitions between higher states. Consequently, the two potentials discriminate between transitions involving the ground states and those involving higher states.

Keywords: photoionization cross section, quantum dot, confining potential, donor impurity

1 INTRODUCTION

Realization of nanostructures of different dimensions and geometries has been beneficial to the scientific community and the world at large, because of applications and possible applications in a wide range of disciplines like biomedicine [1], optoelectronics [2] and radiation detection [3], among others. The mushrooming of different techniques to obtain a plethora of nanostructures has prompted both theoretical and experimental research into these structures.

Among quantum phenomena probed, photionization is equally appealing. The effect of the anisotropy of quantum confinement on photoionisation cross section (PCS) has been probed, and was shown to be appreciable for certain degree of anisotropies [4]. The influences of electric fields and intense laser fields were also reported on, revealing a blueshift of the peak of the PCS with increasing laser strength [5]. PCS of a trion (a hole or an electron bound to an exciton) was probed by Xie, and the effect that pressure, parabolic confinement frequency and hole mass has on it [6]. Apart from parabolic confinement, the other confining potential topography studied is the power-exponential [7]. PCS of quantum rings has also been reported, wherein influences of the inner radius [8] and of magnetic field [9, 10] on the PCS are scrutinized. The role that the impurity position plays in modifying the PCS in a core-shell nanodot has been investigated [11]. In this communication, effects of the cup-like and hill-like parabolic confining potentials on the PCS for a spheroidal quantum dot (SQD) are investigated.

2 THEORETICAL MODEL

2.1 Photoionization cross section

The system investigated is one of a spheroidal quantum dot (SQD) which maybe a *GaAs* material embedded in a $GaAl_xAs_{\{1-x\}}$ matrix. The potentials inside the spherical dot assume a parabolic geometry. A bi-parabolic (cup-like) potential is contrasted with an inverse lateral bi-parabolic (hill-like) potential, each superimposed on an infinite spherical square well (ISSW). Photoionization, which can be regarded as the probability that a bound electron can be liberated by some appropriate radiation [5], is given by [5-9]

$$\sigma_{lm} = \sigma_o \hbar\omega \sum_f \left| \langle f | \vec{r} | i \rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right), \tag{1}$$

where $\hbar\omega$ is the photon energy and $\sigma_o = \frac{4\pi^2 \alpha_{FS} n}{3\varepsilon}\left(\frac{E_{in}}{E_{av}}\right)^2$.

E_{in} is the effective incident electric field and E_{av} is the average electric field in the dot of refractive index n. E_i and E_f are energies associated with initial and final eigen states $| i \rangle$ and $| f \rangle$, respectively. $\left|\langle f | \vec{r} | i \rangle\right|$ is the usual interaction integral coupling initial states to final states, α_{FS} the fine structure constant and $\vec{r}$ is position vector. The wave functions are obtainable as solutions to the Schrödinger equation with the form $\Psi_{lm} = C_{lm} Y_{lm}(\theta,\varphi)\chi(\rho)$, dependent on the potential, where $\chi(\rho)$ is the radial component of the wave function satisfying the Schrödinger equation

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$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\chi(\rho)}{d\rho}\right) + \left\{\frac{2\mu}{\hbar^2}\left[E_{lm}+\frac{k_e e^2}{\varepsilon\rho}-V(\rho)\right]-\frac{l(l+1)}{\rho^2}\right\}\chi(\rho)=0, \quad (2)$$

with μ being the effective mass of electron (of charge *-e*), k_e the Coulomb constant and ε the dielectric constant of the SQD. The orbital momentum quantum number, $l(l=0,1,2,...)$, quantifies angular momentum of an electron. $Y_{lm}(\theta,\varphi)$ is the usual spherical harmonic, *m* being is magnetic quantum number and C_{lm} is normalization constant.

2.2 The Wave Functions

2.2.1. The bi-parabolic (cup-like) potential

2.2.1.1 In the presence of the impurity

Solution to the Schrödinger equation for the bi-parabolic potential

$$V(\rho)=\frac{1}{2}\mu\omega_o^2(\rho-R/2)^2, \quad \infty \ \ elsewhere, \quad (3)$$

is in terms of the Huen Biconfluent function [12, 13];

$$\chi(\rho)=e^{g_1(\rho)}\rho^{|l|}HeunB(|2l+1|,\alpha,\beta,\gamma,g_2(\rho)), \quad (4)$$

with

$$\alpha=iR\sqrt{\frac{\mu\omega_0}{\hbar}},\ \beta=-\frac{2E_{lm}}{\hbar\omega_0},\ \gamma=-\frac{4ik_e e^2}{\varepsilon\hbar}\sqrt{\frac{\mu}{\hbar\omega_0}}$$

$$g_1(\rho)=\frac{\mu\omega_0}{2\hbar}(\rho-R)\rho, \text{ and } g_2(\rho)=-i\sqrt{\frac{\mu\omega_0}{\hbar}}\rho. \quad (5)$$

Requiring that electron wave function should vanish at the walls of the SQD avails the energy spectrum for an electron in a SQD with an intrinsic bi-parabolic potential as

$$E_{lm}=-\frac{\beta_E}{2}\hbar\omega_0, \quad (6)$$

where β_E is the value of β that satisfies the condition

$$HeunB(|2l+1|,\alpha,\beta_E,\gamma,g_2(\rho))=0. \quad (7)$$

2.2.1.2 Neglecting the donor impurity

Disregarding the electron-impurity interaction, the Schrödinger equation is still solvable in terms of the Heun Biconfluent function with parameters being identical to those for this potential in the presence of the donor impurity except for $\gamma=0$ and $\beta^0=-\frac{2E_{lm}^0}{\hbar\omega_0}$, availing the energies without the Coulombic interaction as

$$E_{lm}^0=-\frac{\beta_E^0}{2}\hbar\omega_0, \quad (8)$$

where β_E^0 is the value of $\beta=\beta^0$ that satisfies the condition found in equation (7).

2.2.2 The inverse lateral bi-parabolic (hill-like) potential

2.2.2.1 In the presence of the impurity

This potential is maximum at the centre of the SQD, and decreases parabolically towards the walls;

$$V(\rho)=\frac{1}{2}\mu\omega_o^2(R\rho-\rho^2), \quad \infty \ \ elsewhere. \quad (9)$$

Radial component of the Schrödinger equation is also solvable in terms of the Heun Biconfluent function (4) but with

$$\alpha=R\sqrt{\frac{\mu\omega_0}{i\hbar}},\ \beta=\frac{\mu\omega_0^2R^2-8E_{lm}}{4i\hbar\omega_0},$$

$$\gamma=\frac{4k_e e^2}{\varepsilon\hbar}\sqrt{\frac{-\mu}{i\hbar\omega_0}},\ g_1(\rho)=\frac{\mu\omega_0}{2i\hbar}(R-\rho)\rho \quad \text{and}$$

$$g_2(\rho)=\sqrt{\frac{-i\mu\omega_0}{\hbar}}\rho. \quad (10)$$

Application of the boundary conditions at the walls of the QD avails the energy spectrum as

$$E_{lm}=\frac{1}{8}\mu\omega_0^2R^2-\frac{i\beta_E}{2}\hbar\omega_0, \quad (11)$$

where β_E is the value of β that satisfies the condition set in equation (7).

2.2.1.2 Neglecting the donor impurity

In this case, the parameters have the same expressions as those for this potential in the presence of the impurity (Eq.

10) except for $\gamma = 0$ and $\beta^0 = \frac{\mu\omega_0^2 R^2 - 8E_{lm}^0}{4i\hbar\omega_0}$, hence the energy associated with the hill-like potential without the Coulombic interaction can be cast in the form

$$E_{lm}^0 = \frac{1}{8}\mu\omega_0^2 R^2 - \frac{i\beta_E^0}{2}\hbar\omega_0, \quad (12)$$

β_E^0 still being the value of $\beta = \beta^0$ that satisfies the condition stipulated in equation (7).

3 DISCUSSIONS

This section is dedicated to discussions and analysis of the results. Parameters used in the computations are $\mu = 0.067m_e$, m_e being the free electron mass and $\varepsilon = 12.5$, pertaining to GaAs nano dots. The geometries of the confining potentials are illustrated in Fig 1, where $\kappa = \left(2/\mu\omega_0^2 R^2\right)$, which depicts the influence strengths of these potentials on the radial component of the ground state electron wave function. By virtue of the fact that the

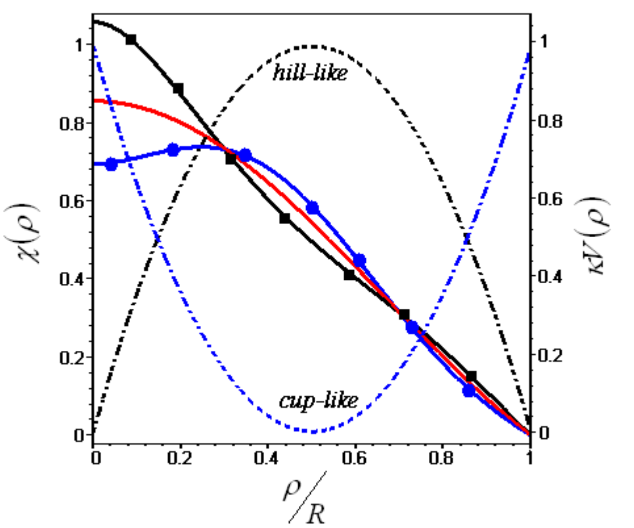

Figure 1: Effects of the two parabolic potentials (which are the dash-dotted curves) on the ground state radial electron wave functions across a SQD. The plot marked with dots corresponds to the ground state wave function in an SQD with a cup-like potential while the one marked with squares is associated with the hill-like potential, each of strength $\hbar\omega_0 = 15meV$. The solid unmarked plot is the ground state radial wave function in an SQD with a purely ISSW ($\hbar\omega_0 = 0meV$).

cup-like parabolic potential is maximum at the centre and at the walls of the SQD, it reduces the ground state electron wave function at those points, and merely tightens electron wave functions of excited states around a radial distance half the radius of the SQD. The hill-like potential, contrastingly, is maximum at the radial distance half the radius of the SQD ($0.5R$), and thus dwindles electron wave functions at this radial distance, and enhances wave functions elsewhere.

The hill-like (cup-like) potential perturbs the excited states (ground state) more than it does the ground state (excited states). This gives the hill-like (cup-like) potential the propensity to enhance (dwindle) transition energies $\Delta E = E_f - E_i$ (Fig 2). As such, intensification of the hill-like (cup-like) potential blue-shifts (red-shifts) the peaks of the PCS (Fig 3).

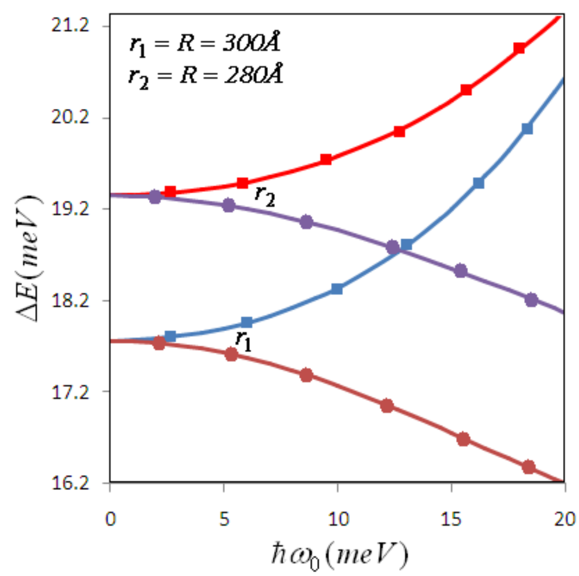

Figure 2: Energy differences between the ground state (s) and the first excited state (p) as functions of strengths of the parabolic potentials for the indicated radii of the SQD; the plots marked with dots are associated with the cup-like parabolic potential while those marked with squares are associated with the hill-like parabolic potential.

The energy difference between the s and p states in an SQD of radius 300Å is in the vicinity of 17.762 meV in the absence of the parabolic potentials ($\hbar\omega_0 = 0meV$). Figure 4 shows the dependence of the normalized PCS for such a spheroidal quantum dot on strengths of the parabolic potentials. If the beam energy of excitation is lower than the transition energies, then the cup-like potential can be used to capacitate photoionization by increasing its intensity until the transition energies are coincident with the beam energy. This enhances the PCS to a peak at the energy of resonance. The PCS will decrease with intensification of the hill-like potential for beam energy lower than excitation energy, since the potential enhances transition energy. Conversely, intensification of the cup-like potential will merely diminish the PCS for beams energies larger than excitation energy, while the hill-like potential will increase transition energies until they equal the beam energy, thereby intensifying the PCS.

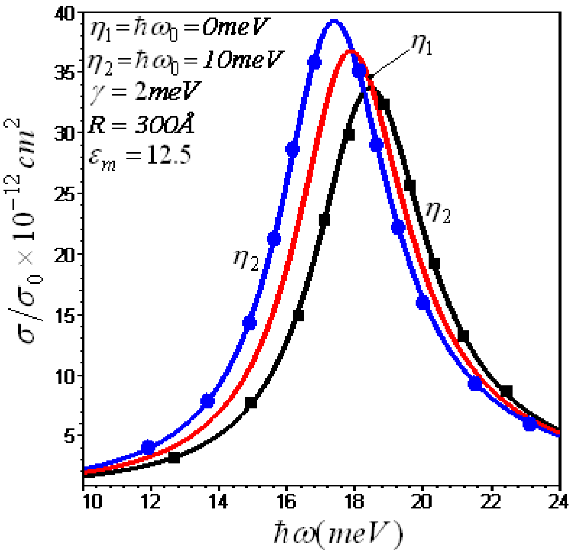

Figure 3: Dependence of the normalized PCS on the beam energy for an ISSW ($\hbar\omega_0 = 0meV$) and for the cup-like (plot with dots) and the hill-like (plot with squares) parabolic potentials superimposed on the ISSW, each of strength $\hbar\omega_0 = 10meV$.

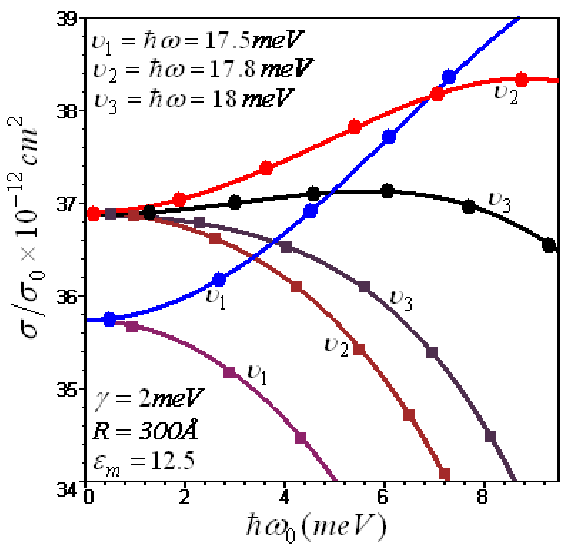

Figure 4: Variation of the normalized PCS with strengths of the cup-like (curves with dots) and the hill-like (marked with squares) parabolic potentials for the different beam energies of excitation.

Because transition energy scales inversely with the radius of the SQD, the two potentials afford us the ability to adjust transition energies without necessarily having to tamper with the dimensions of SQD. This is advantageous in cases where excitation energy is to have a specific value which an ISSW SQD of the required radius may not have.

4 CONCLUSIONS

Analytical expressions of electron wave functions in a spheroidal quantum dot with and without a centred donor impurity have obtained and utilized to probe the effects of the cup-like and hill-like parabolic potentials on the PCS. The ability of these potentials to modify transition energies without altering the sizes of SQDs avails nanotechnology immense control over tunability of these structures, through appropriate nano patterning.

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